

Solvation Properties of Fluorinated Molecules

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The use of liquid fluorinated species as solvents attracts considerable attention from different fields of application: in biomedicine (as in vivo gas carriers, ultrasound contrasting agents, etc), as solubility enhancers in supercritical carbon dioxide or as clean solvents in reaction media (immiscible in both aqueous and organic phases). A double approach, based on solubility experiments and in free energy calculations by computer simulation, is followed to provide insights about the structure of the solutions containing fluorinated species and about the solute-solvent interactions, to model phase equilibria and to calculate solubilities and partition coefficients of solutes between fluorinated and other phases. The solubility of several gases in different liquid fluorinated molecules (linear and cyclic perfluorinated alkanes, brominated perfluorocarbons and semifluorinated alkanes) are measured using isochoric or isobaric saturation methods in which the solubility is determined from the quantity of gas dissolved in an accurately known volume of solvent, at constant temperature. Quantum mechanical calculations and molecular dynamics simulations are used to formulate new force fields for families of fluorinated molecules such as brominated perfluorocarbons and hydrocarbon-fluorocarbon diblocks (semifluorinated alkanes). Standard Gibbs energies of solvation, and from there Henry's law coefficients, are calculated by appropriate free energy routes (test-particle insertion, thermodynamic integration). The Henry's law coefficients or partition coefficients obtained from simulation are compared with experimental values. Structural details such as the distribution of cavities in the solvent are analyzed and the nature of the solute-solvent interactions is investigated.